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Title:	LDRD-DR midterm review - High-order hydrodynamic methods for exascale computing
Author(s):	Morgan, Nathaniel Ray Burton, Donald E.
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LDRD-DR midterm review - High-order hydrodynamic methods for exascale computing

Principle Investigators:

Nathaniel Morgan and Donald Burton

Co-investigators:

Konstantin Lipnikov, Xiaodong Liu, Evan Lieberman, Mike Berry, Vincent Chiravalle, DJ Luscher, Rob Lowrie, and Misha Shashkov

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X: Computational Physics

Los Alamos National Laboratory

Motivation and Background Information

Algorithm research is essential for efficiently computing on emerging architectures and moving towards exascale computing

- **Key observations:**
  - The LLNL finite element method (FEM) has high compute intensity
  - FEM scales better than the finite volume Lagrangian staggered grid hydrodynamic (SGH) method
    - FEM is faster beyond 256 cores (16 nodes)
    - FEM is more accurate than the SGH method
  - High-order FEM has the same runtime as low-order FEM with the same number of degrees of freedom (DOFs)

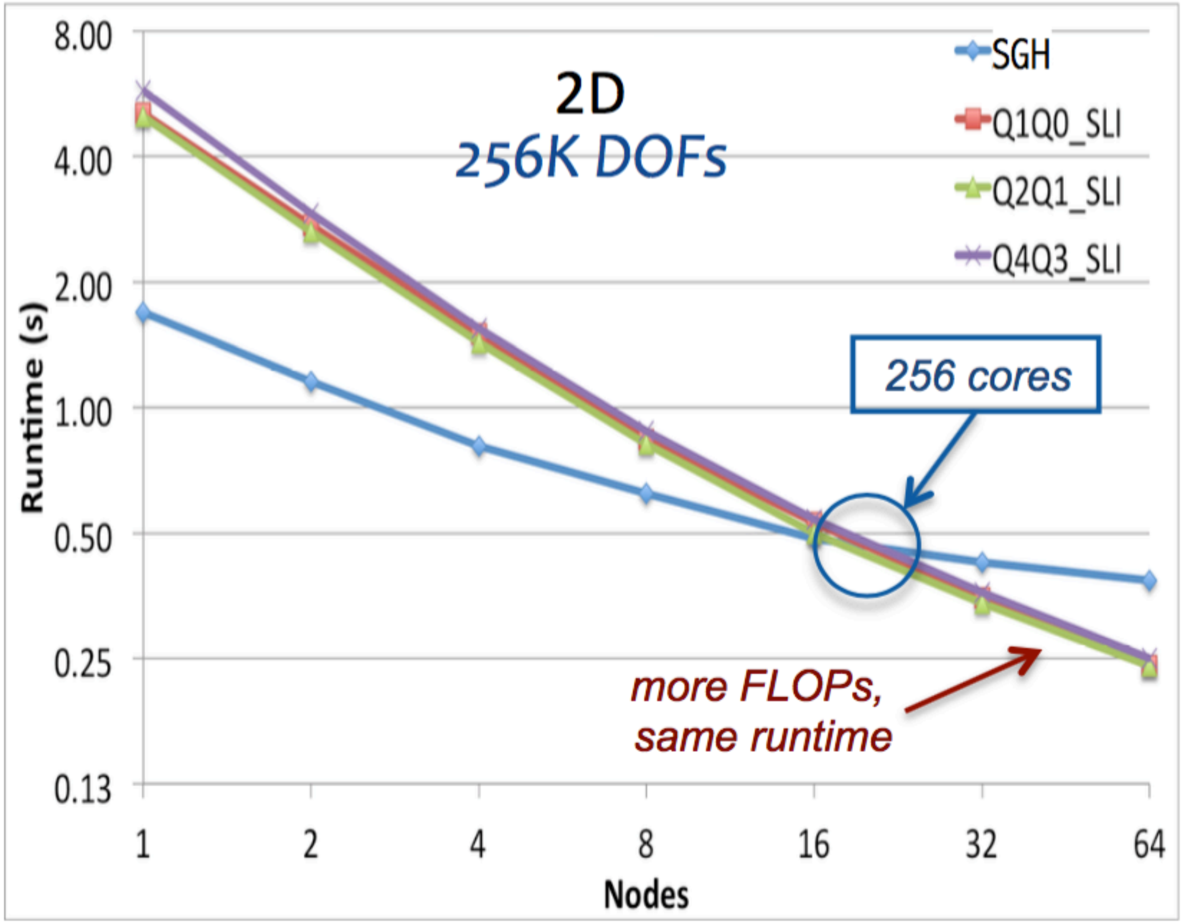
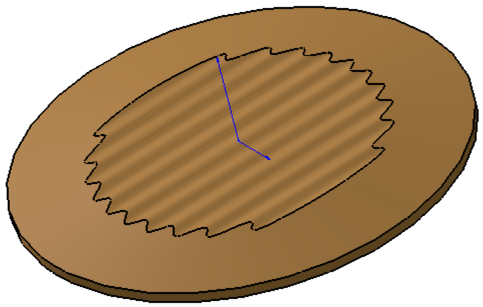


Fig: *A scaling study performed by LLNL using the Sedov blast wave [1]*

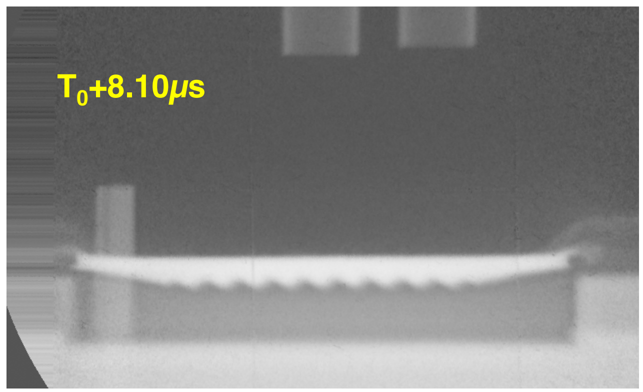
1. T. Kolev, R. Anderson, T. Brunner, J. Cerveny, V. Dobrev, A. Grayver, I. Karlin, R. Rieben, BGSIAM15 Conference, 2015

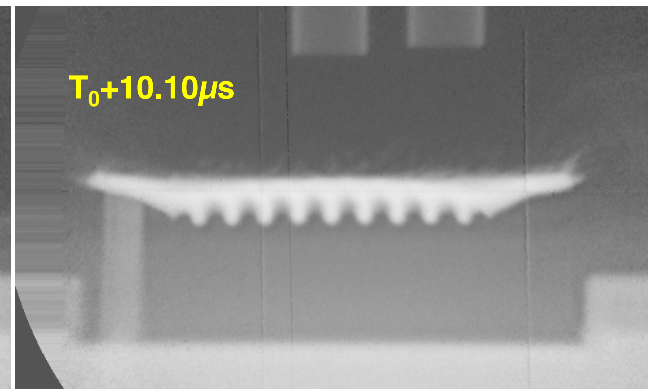
Many laboratory missions require accurate simulations of vorticity ranging from dynamic material experiments to ICF

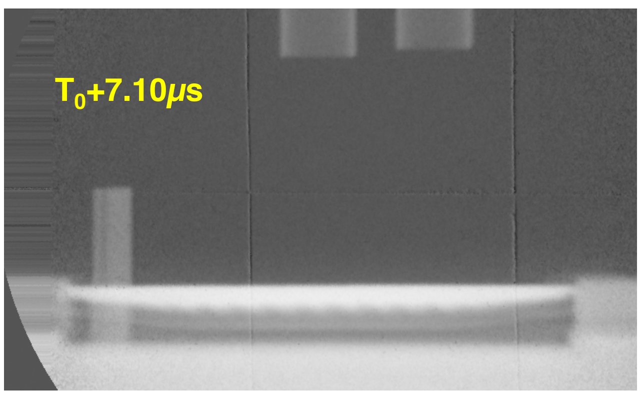
- **Consider the PRad experiments for investigating "The effect of microstructure on Rayleigh-Taylor instability growth in solids" [1].**
  - **1.5 mm thick Cu plate with a 55 μm perturbation is driven by a high explosive**

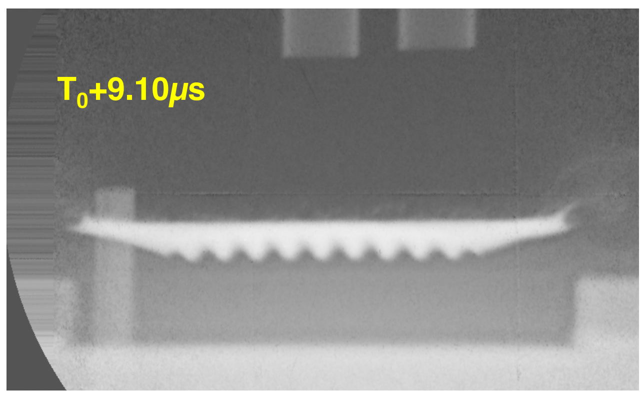


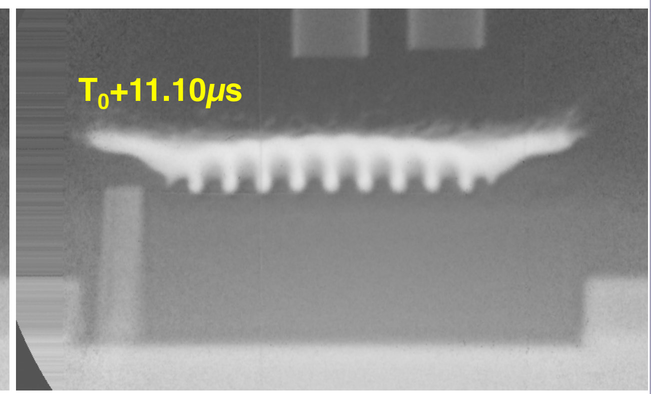
20 mm diameter





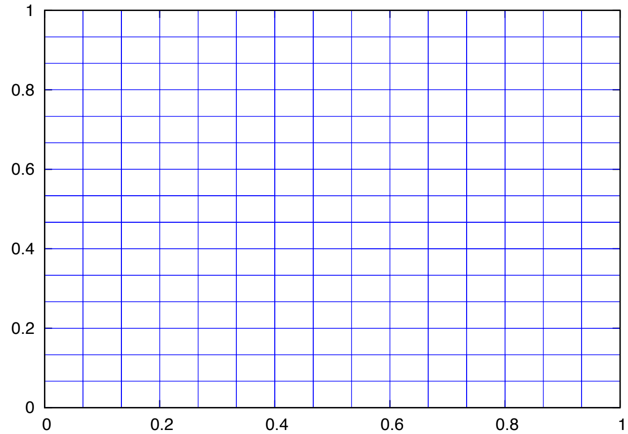




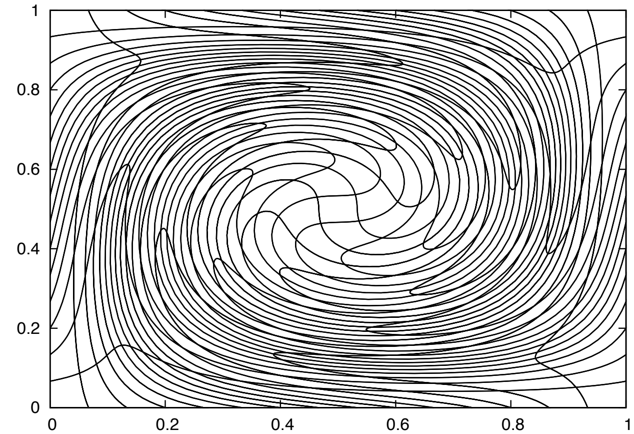


1. R.T. Olson, E.K. Cerreta, C. Morris, A.M. Montoyam, F.G. Mariam, A. Sauders, R.S. King, E.N. Brown, G.T. Gray, and J.F. Bingert, APS-SSM & AIRAPT-24 Joint Conference, Seattle, WA July, 2013.

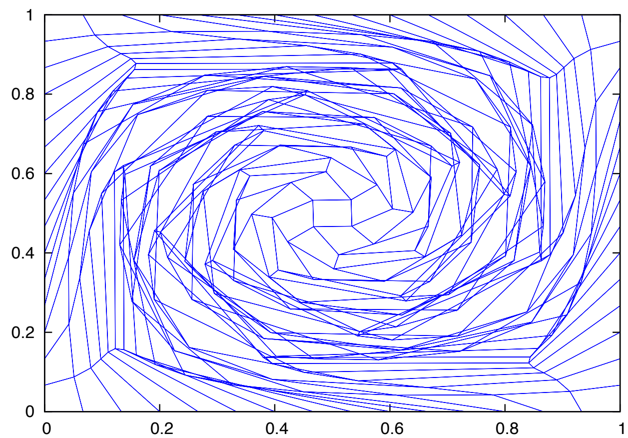
Lower-order algorithms have difficulties accurately simulating complex flows and have poor compute intensity



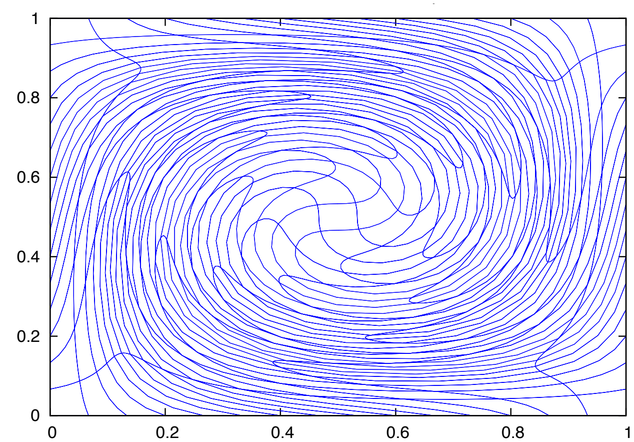
(a) Initial mesh



(b) Analytic mesh deformation



(c) Standard linear elements tangle



(d) Cubic elements can bend

Fig: *High-order elements better capture the details of the vortical flow compared to linear elements. Calculations are of the Rider-Kothe vortex and the time corresponds to 1 rotation of the center element.*

We propose to develop the *first* Lagrange+remap ALE discontinuous Galerkin (DG) hydrodynamic method on high-order elements for simulating gas and solid dynamics

- **Previous Lagrangian DG research is very sparse and very limited in focus**
  - All research to date has focused on single material gas dynamics
    - Researchers in China [1, 2] studied 2D Lagrangian motion with linear element faces
    - Researchers in France [3] investigated 2D Lagrangian motion on linear and quadratic element faces, but the method had spurious mesh motion on the Sedov blast wave problem with a quadratic element (discussed on next slide)
  - Evolving curved element faces in a stable manner with Lagrangian DG was an unsolved problem
  - The existing DG methods do not support the models, algorithms, and capabilities required to simulate most programmatic applications at LANL
- **The DG method requires extensive research and development to simulate solid dynamics**

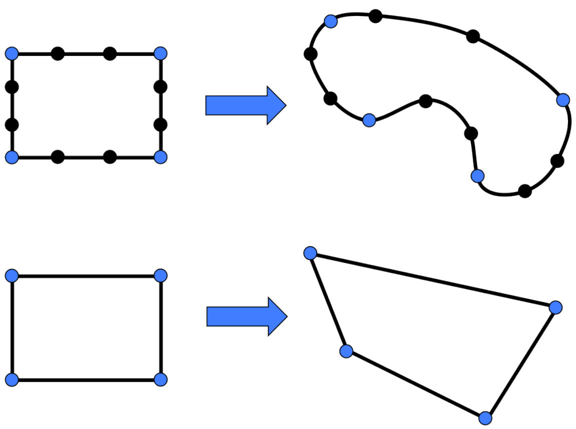


Fig: *High-order elements (top) can bend, whereas, linear elements (bottom) are stiffer*

1. Z. Jia and S. Zhang, Journal of Computational Physics, 2011;230:2496-2522.
2. Z. Li, X. Yu, and Z. Jia, Computers and Fluids, 2014;96:152-164.
3. F. Vilar, P-H. Maire and R. Abgrall, Journal of Computational Physics, 2014;276:188-234.

Application of curved elements to Lagrangian hydrodynamics is an emerging field of study

- **Vilar et. al. [1] are the only team to research high-order elements with Lagrangian DGH**
  - Spurious mesh motion was present in the calculations of the Sedov blast wave problem in [1]

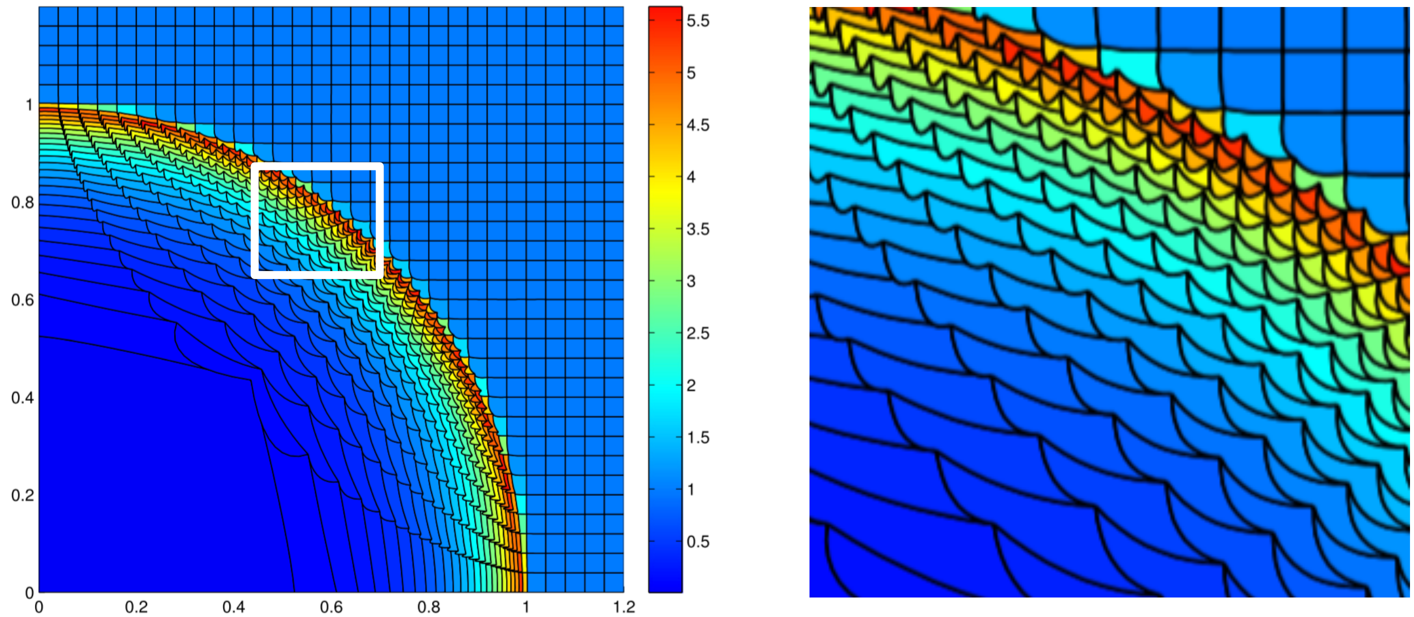


Fig: *Numerical instabilities with curved elements in 2D XY coordinates are shown. Images were taken from [1]*

1. F. Vilar, P-H. Maire and R. Abgrall, Journal of Computational Physics, 2014; 276:188-234.

Programmatic impact

DG methods possess the key criteria for *efficiently* computing on emerging architectures and moving towards exascale

- **Algorithm requirements:**
  - High FLOPS per memory access time
  - Data locality
  - Reduce the wall-clock time that it takes to reach the required level of accuracy
- **Previous research demonstrates the merits of high-order methods**
  - Research in [1] achieved order-of-magnitude performance gains on GPUs with a high-order DG method for solving Maxwell's electro-magnetic equations in 3D for linear, isotropic, and time-invariant materials
  - A DG approach applied to seismic wave propagation achieved order of magnitude speed-ups on GPUs [2]
- **Eulerian nodal and modal DG methods were shown to perform very well with GPUs [3]**

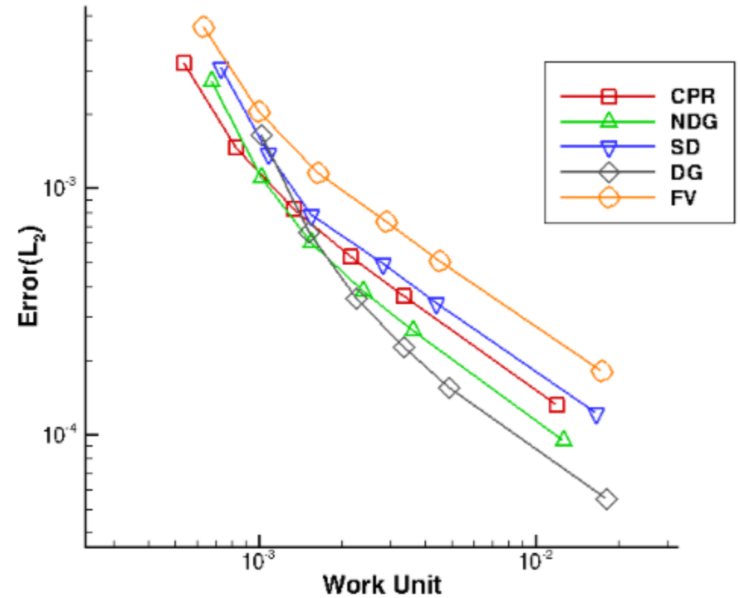


***Fig:** Results from [3] for 2nd-order accurate methods demonstrate the merits of using higher flop methods on GPUs*

1. A. Klockner, T.Warburton, J. Bridge,and J. Hesthaven, Journal of Computational Physics, *2009;228:*7863-7882.
2. D. Mu, P. Chen, and L. Wang, Earth Science 2013;26(6):377-393
3. Zimmerman, B. J, Regele, J. D. and Wie, B., A Comparative Study of 2D Numerical Methods with GPU Computing, arXiv:1709.01619, pp. 1-24, 2017.

Additional speed-ups are achievable with high-order algorithms

- **The calculation time for a 3D hydrodynamic method typically scales as $1/dx^4$ so accuracy improvements can enable coarser mesh resolutions (dx increases) that reduce calculation time**
- **On a 3D vortex problem, a high-order finite volume method [2] could achieve 20X speed-ups for the same accuracy; alternatively, the errors could be reduced by 100X for the same calculation time**

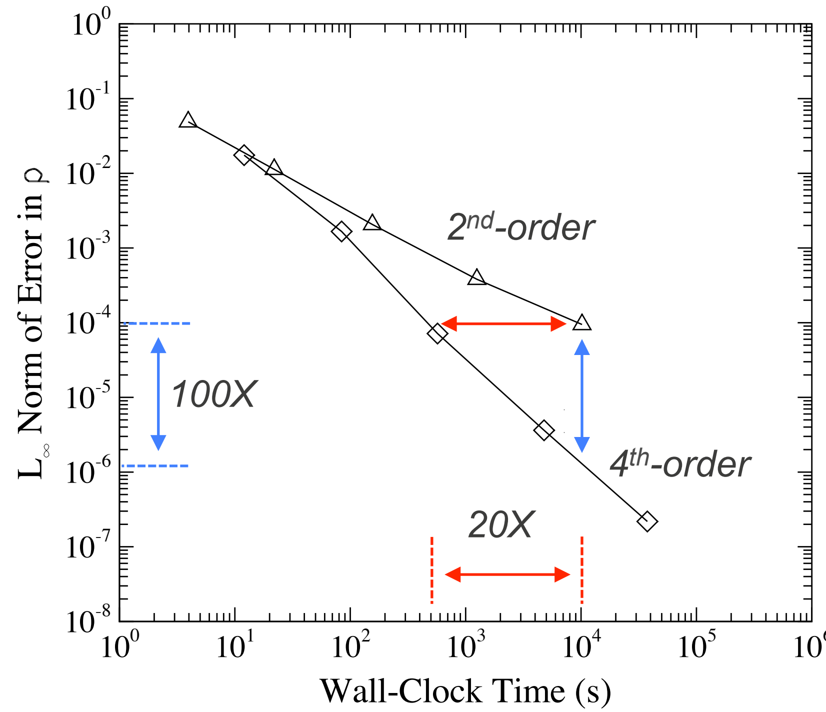


Fig: *Results from [2] demonstrate the merits of using high-order methods*

1. A. Klockner, T.Warburton, J. Bridge,and J. Hesthaven, Journal of Computational Physics, *228,* 7863 (2009).
2. M. Charest, T. Canfield, N. Morgan, J. Waltz, and J. Wohlbier, Computers & Fluids, 2015; 114:172-192.

High-order elements are essential for large deformation problems with contact surfaces

- **Eulerian and Arbitrary Lagrangian Eulerian (ALE) methods cannot accurately simulate sliding and impacting surfaces**
- **A Lagrangian method with high-order elements is beneficial in many contact-surface problems ranging from shaped-charge experiments to car crash safety simulations**

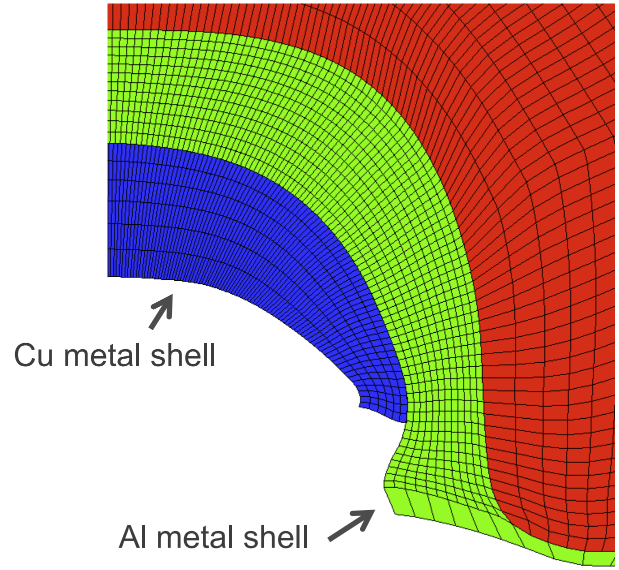


***Fig:** A shaped charge experiment*

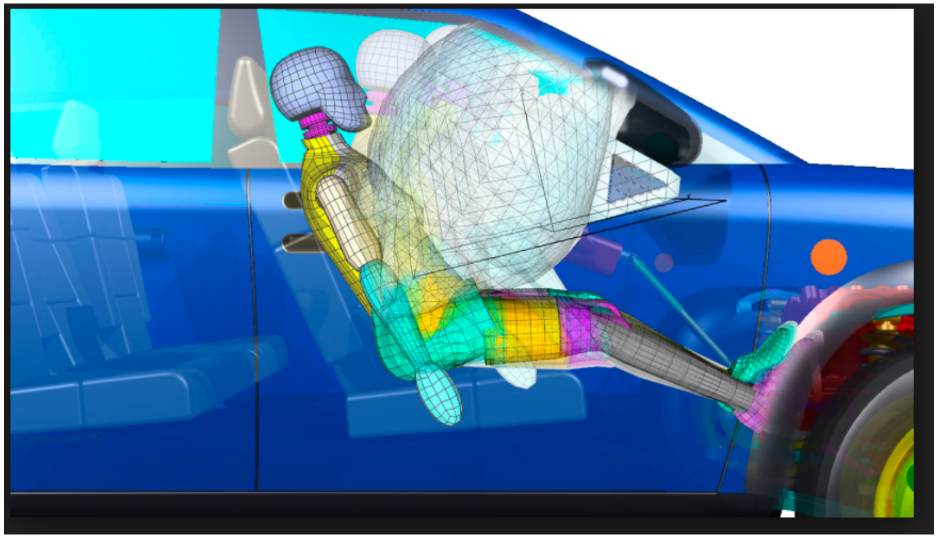


***Fig:** Occupant safety simulation*

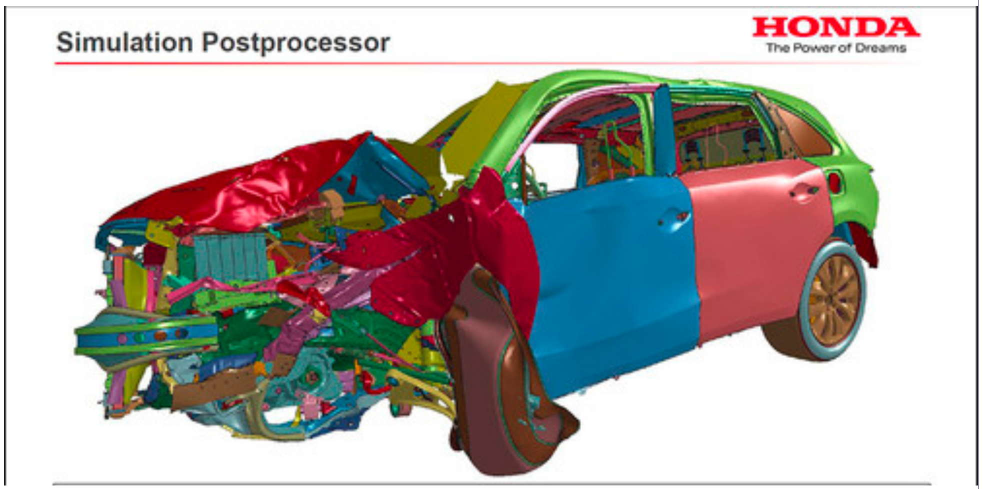
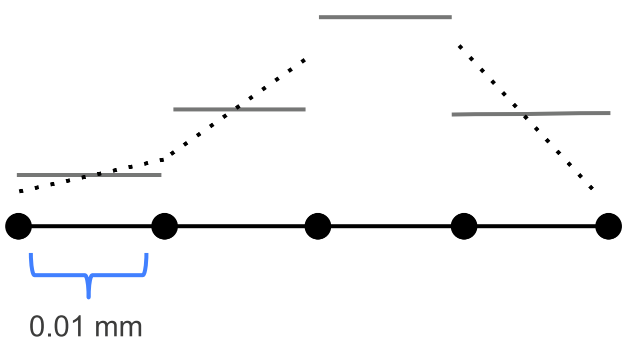


***Fig:** A car crash simulation*

High-order FE and DG methods can bridge physics length scales

- **The DG method replaces a finely resolved mesh with a high-order Taylor-Series polynomial**
  - DG potentially can simulate fine-scale physics with a larger mesh size by evaluating the physics models at the Gauss quadrature points

$$\text{cost}_{FV} = \frac{N_{cells}}{\Delta t} = \left(\frac{c}{\Delta x_{small}}\right)\frac{1}{\Delta x_{small}^{3}} = \frac{c}{\Delta x_{small}^{4}}$$

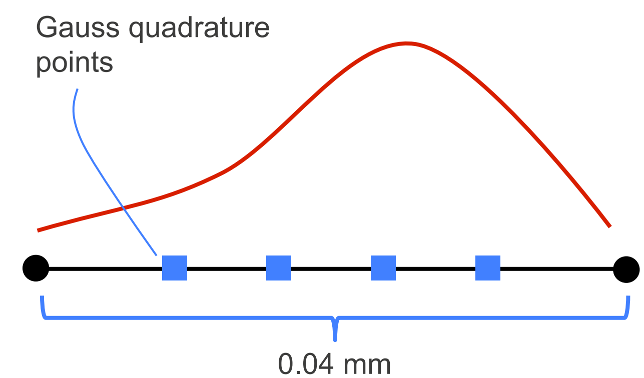


The standard finite volume (FV) method

VS.

~256X cheaper

$$\text{cost}_{DG} = \frac{N_{cells}}{\Delta t} = \frac{c}{4^4\,\Delta x_{small}^{4}} = \frac{c}{256\Delta x_{small}^{4}}$$



A high-order DG method

High-order FE and DG methods may enable reactive burn calculations at more feasible mesh resolutions

- **Reactive burn simulations can require 10μm resolution**
- **HE reactions can be coupled to DG at the Gauss points**

Mass: $$\mathbf{M}^{kl} = \int_{w(t)} \rho \psi^k \psi^l \, dw$$

Momentum: $$\mathbf{M}^{kl} \frac{d\mathbf{u}^l}{dt} = \oint_{\partial w(t)} \psi^k \mathbf{n} \cdot \boldsymbol{\sigma}^* da - \int_{w(t)} \left(\nabla \psi^k\right) \cdot \boldsymbol{\sigma} \, dw$$

Total energy: $$\mathbf{M}^{kl} \frac{d\boldsymbol{\tau}^l}{dt} = \oint_{\partial w(t)} \psi^k \mathbf{n} \cdot \boldsymbol{\sigma}^* \cdot \mathbf{u}^* da - \int_{w(t)} \left(\nabla \psi^k\right) \cdot \left(\boldsymbol{\sigma} \cdot \mathbf{u}\right) dw + \int_{w(t)} \psi^k E_{HE} \, dw$$

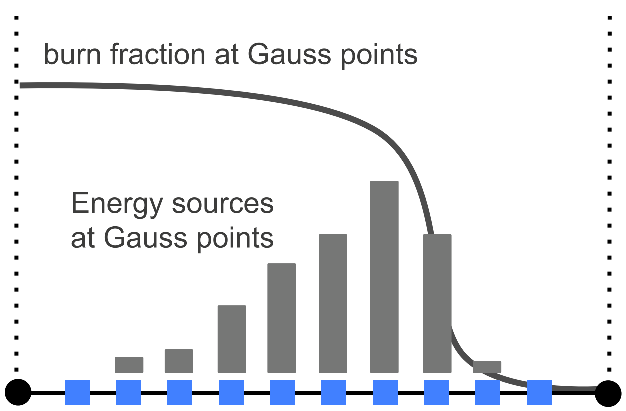
$$\boldsymbol{\sigma} = -p\mathbf{I}$$

$$p = EOS\left(\rho, e\right)$$

E_{HE} = HE energy source

$$\int_{w(t)} E_{HE} \, dw \approx \sum_{g \in \Omega} \psi^k(\xi_g) E_{HE}(\xi_g) j_g \Omega_g$$

$B_f(\xi = -1) = 1$



$B_f(\xi = 1) = 0$

Gauss quadrature points "g"

Summary

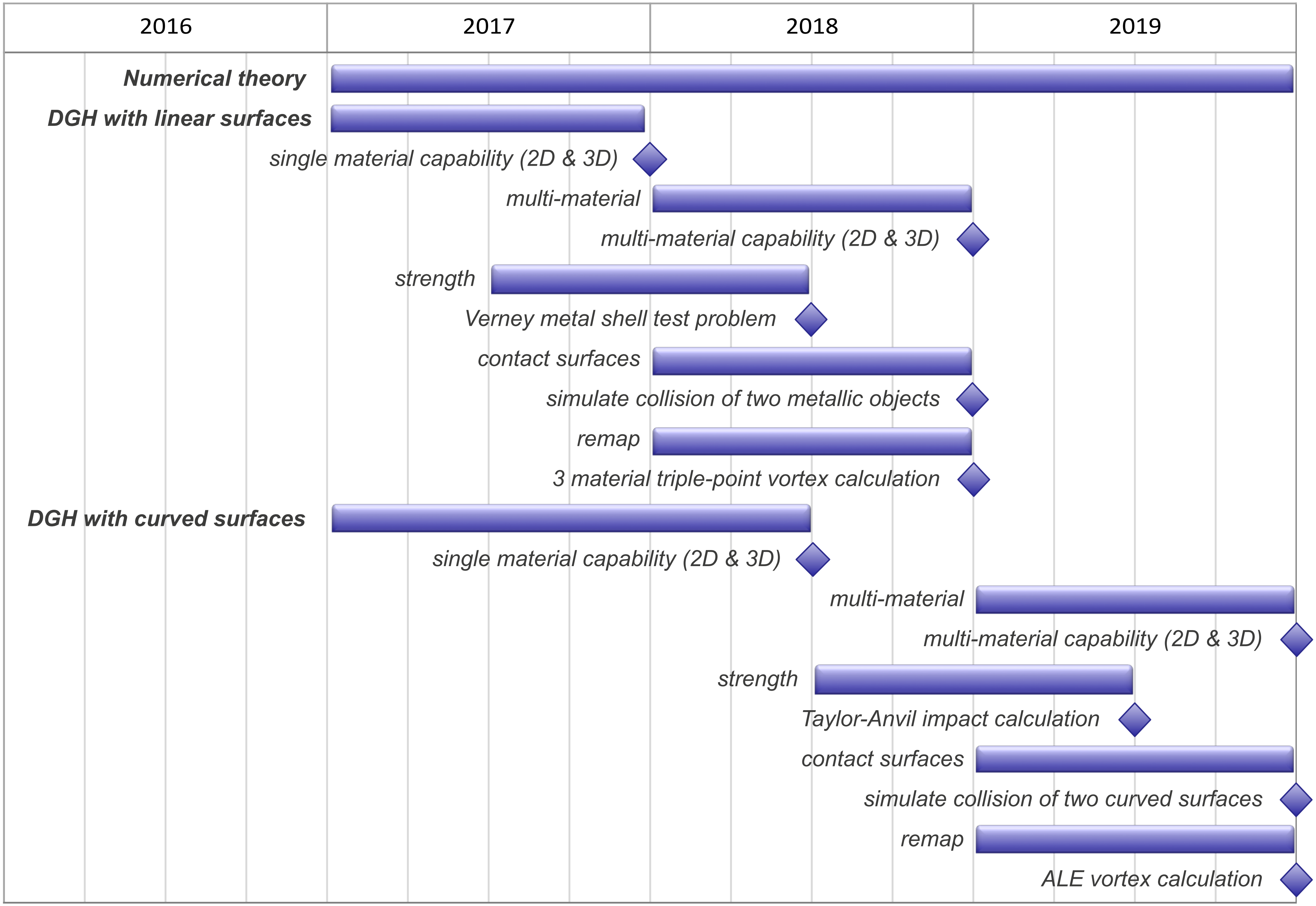
The LDRD-DR research is on schedule and yielding novel methods

- **New 2D XY and RZ Lagrangian DG methods were developed**
  - Conservative modal and nodal density evolution approaches
  - An accurate limiting approach for Lagrangian DG methods
  - The first 2D RZ Lagrangian DG method
- **A 2D/3D compatible Lagrangian DG method was developed that uses piecewise maps to the initial coordinates**
  - The first 3D Lagrangian DG calculations and valid for polytopal elements
  - The first compatible DG evolution equations
- **A new Lagrangian DG method for solid dynamics**
  - The first Lagrangian DG method with strength
- **A new DG remap method for 2D/3D polytopal elements**
  - The first modal DG remap for polytopal elements
- **Methods were created to ensure stable Lagrangian DG solutions on higher-order elements**
  - Smooth mesh motion on strong shocks with collocated hydrodynamic methods

The research team is documenting and presenting the DG work

- **Journal papers**
  - X. Liu, N. Morgan, and D. Burton, *A Lagrangian discontinuous Galerkin hydrodynamic method*, In review
  - N. Morgan, X. Liu, and D. Burton, *Reducing spurious mesh motion in Lagrangian finite volume and discontinuous Galerkin hydrodynamic methods*, In review
  - E. Lieberman, N. Morgan, DJ Luscher, D. Burton, A higher-order Lagrangian discontinuous Galerkin hydrodynamic method for elastic-plastic flows, In review
  - V. Chiravalle and N. Morgan, *A 3D Lagrangian cell-centered hydrodynamic method with higher-order reconstructions for gas and solid dynamics*, to be submitted
  - T. Wu, M. Shashkov, N. Morgan, H. Luo, and D. Kuzmin, *An updated Lagrangian discontinuous Galerkin hydrodynamic method for gas dynamics*, to be submitted
  - X. Liu, N. Morgan, and D. Burton, *A cell-centered Lagrangian discontinuous Galerkin hydrodynamic method in two-dimensional cylindrical geometry*, to be submitted
  - Other papers are in progress *e.g.,* a DG remap paper, and a 2D/3D compatible Lagrangian DG paper
- **Conference papers**
  - X. Liu, N. Morgan, and D. Burton, *A Lagrangian cell-centered discontinuous Galerkin hydrodynamic method for 2D Cartesian and RZ axisymmetric coordinates*, AIAA 2018
  - N. Morgan, X. Liu, and D. Burton, *A Lagrangian discontinuous Galerkin hydrodynamic method for higher-order triangular elements*, AIAA 2018
- **Conference**
  - N. Morgan, X. Liu, and D. Burton, *Reducing spurious motion in Lagrangian hydrodynamics*, presentation, MultiMat 2017
  - V. Chiravalle and N. Morgan, *A limiting approach for higher-order Lagrangian cell-centered hydrodynamic (CCH) methods,* presentation, MultiMat 2017
  - X. Liu, N. Morgan, and D. Burton, *A Lagrangian cell-centered discontinuous Galerkin (DG) hydrodynamic method*, poster, MultiMat 2017

EXTRA


2016
2017
2018
2019
Numerical theory
DGH with linear surfaces
single material capability (2D & 3D)
multi-material
multi-material capability (2D & 3D)
strength
Verney metal shell test problem
contact surfaces
simulate collision of two metallic objects
remap
3 material triple-point vortex calculation
DGH with curved surfaces
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